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## Numerical modeling of bacterium-surface interaction by applying DEM

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### Abstract

In order to understand the behaviour system of the bacteria it is important understand the behaviour of a single bacteria. The suspension forming bacteria may be considered as system of living active ultrafine particles (size 1  $\mu\text{m}$ ). Present investigation addresses to the simulation of the *S. aureus* bacterium-surface interactions in a framework of the Discrete Element Method (DEM). Bacterium is of the spherical shape, while the glass surface is flat and considered as elastic. In this work the theoretical model for bacteria is similar to that used for the ultrafine size stiff particles. We investigate the behaviour of the active particle by applying two known Derjaguin, Müller, Toporov (DMT) [1] and Derjaguin, Landau, Verwey, Overbeek (DLVO) [2, 3] models, which are used for simulation of ultrafine size objects. These models are enhanced by applying suggested dissipation mechanism related to the adhesion. It was assumed that energy can be dissipated and the force-displacement hysteresis can occur through the adhesion effect, where an amount of dissipated energy is fixed and independent on initial kinetic energy. This force-displacement hysteresis was observed at the physical experiments with bacteria provided by the means of the atomic force microscopy (AFM), Ubbink and Schär-Zammaretti (2007) [4]. It was illustrated that the presented adhesive-dissipative model, which applies DEM, offers the opportunity to capture dissipation effect during the contact. The numerical experiments confirm that force-displacement plots exhibit hysteresis typical to those which are observed in AFM experiments. This model can be useful for numerical simulation of interaction of bacterium to the substrate.

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## 1. Introduction

The motions of bacteria through the air and collisions with the surfaces of adjacent biological or inorganic elements are processes contributing propagation of human infections, caused by pathogenic bacterium. The human sneezing, coughing, as well as action of devices such as humidifiers, air conditioning systems could be a reason of this motion. Transmission of Bacteria through the air can be interpreted as motion of particles. This phenomena was observed by Tang et al. (2006) [5], Todd and Belteton (2014) [6]. Different approaches can be applied for simulation of bacteria motions. The diffusion and chemotaxis of bacterial cells are processes playing a fundamental role for active suspension behaviour and biofilm formation, Šimkus, Baronas, and Ledas (2013) [7]. On the other hand the issue of bacteria interaction with a surface has to be solved by considering mechanical motion described with Discrete Element Method (DEM). In order to understand bacterium behaviour it became interest of interaction nature of bacterium. In this case the bacterium interaction is described by the action of mechanical forces. It should be remarked, that forces of interbacterial interaction are of different nature compared to larger particles which induce coupling of different deformation modes. The model of particles is introduced hereafter for description of beaticles behaviour convention. The normal interaction considered hereafter.

Generally motion of particles, in our case bacteria could be contributed by attractive and repulsive force. The influence of the adhesion is described by the attractive van der Waals force. In this work the theoretical model for bacteria is similar to that used for the ultrafine size stiff particles. We investigate the behaviour of the active particle by applying two known Derjaguin, Müller, Toporov (DMT) and Derjaguin, Landau, Verwey, Overbeek (DLVO) models, which are used for simulation of ultrafine size objects.

Concise review of mechanisms of bacterial adhesion to biomaterial surfaces was made by Yuehuei, Richard and Friedman (1988) [8]. Influence of surface energy was studied by Liu and Zhao (2005) [9]. Theoretical prediction of collision efficiency between adhesion-deficient bacteria and sediment grain surface was made by Dong et al. (2002) [10].

One of main characteristic phenomena caused by adhesion of small size objects like bacteria is process of sticking with interacting surface due to adhesion. *S. aureus* adhesion to different treated titanium surfaces was investigated by Harris and Richards (2004) [11]. The stick of *S. aureus* to mucus components of the respiratory epithelium was investigated by Ulrich et al. (1998) [12].

Roughness of bacterium play role on the influence of van der Waals force, because it is dependent on surface area of interacting surfaces. Roughness of bacteria was investigated by Francius et al. (2008) [13]. *S. aureus* attachment patterns on glass surfaces with nanoscale roughness was investigated by Mitik-Dineva et al. (2009) [14].

The simulation of ultrafine size objects interaction can be described by applying Derjaguin, Landau, Verwey, Overbeek (DLVO) model. This model includes attractive adhesive and repulsive electrostatic double layer forces, which acts at a distance from interacting surfaces. Influence of repulsive electrostatic double layer force on bacteria was investigated by Poortinga et al. (2002) [15]. Abu-Lail and Camesano (2006) [16] investigate the effect of solvent polarity on the molecular surface properties and adhesion of *E. Coli*. The elasticity and molecular surface characteristics of *E. Coli JM109* bacterium were investigated via atomic force microscopy (AFM) in solvents expressing different polarities. Atomic force microscopy of microbial cells was observed by Gaboriaud and Dufrêne (2007) [17]. They observe progresses in sample preparation techniques, while denoted that instrumentation and recording conditions for living cells are still needed to improve the accuracy and reproducibility of force measurements. It is also important to refine treatments currently available to interpret approach force curves recorded on microbial surfaces.

In this paper main attention is given for numerical simulation of interaction of transmitted in air bacterium with a surface. Initially bacterium motion is given by bioaerosol. In most cases, the behavior of bacterium during the contact is treated, however, in a non-unique way, and different attractive-non-dissipative or dissipative, models are used in the numerical analysis. It should be noted that even the simplest adhesion process may be not only reversible; however, it can involve the adhesive dissipation of energy. Therefore, the enhancing of the knowledge of the mechanisms of the energy dissipation due to adhesion forces in the normal direction is the main goal of the present paper.

## 2. Problem Formulation

Pathogenic bacterium is able to travel through the air within aerosol droplets (bioaerosol). The task of this investigation is limited to numerical analysis of the bacteria interaction with a wall. Initially bacterium was dispersed in aerosol droplet. The present task is idealised and limited for investigation of interaction of bacterium with wall surface. The chosen bacterium is *S. aureus*. The mechanism of interaction till now is not well known and even controversial. It is because of different factors which are acting on bacterium during interaction. Normal interaction of bacterium with flat surface is done, using following assumptions. Bacterium is considered as a spherical particle. Interaction with surface is described with normal force components. Attraction force between interacting surfaces is considered as van der Waals forces. Additionally it is taken into account short range interaction and related with adhesion energy dissipation mechanism.

The physical experiments with AFM show force-displacement hysteresis behaviour of the *S. aureus* bacterium, see Touhami et al. (2004) [18], Abu-Lail et al. (2012) [19], Younes et al. (2012) [20]. The problem of the task is to describe and take into account this dissipative behaviour of in this work investigated bacterium. In this work on presented model is based on DLVO and adhesive-dissipative models used for modelling of bacterium interaction. The theoretical basis for bacterium movement simulation is taken from investigations of same size ultrafine particles, Tomas (2007) [21], Jasevičius et al. (2011, 2014) [22, 23]. The goal of this work based on the description and numerical analysis of bacterium adhesive normal interaction with surface. Description of behaviour of bacterium during interaction one of the problem, because it needs energy dissipation correlated with influence of attraction. It is because of ability to stick and create such as structures like biofilms. Energy dissipation in this work is presented as mechanism, which depends on amount of dissipated energy related with adhesion. Bacterium lose energy during unload and detachment as it expected for fine objects see Jasevičius et al. (2011) [21]. Also this mechanism allows describe expected effect of hysteresis for bacterium, observed in real physical experiments. The model is adopted for DEM simulations.

The presented investigation is adhesive-dissipative model, which applies DEM, offers the opportunity to capture dissipation effect during the contact. The numerical experiments confirm that force-displacement plots exhibit hysteresis typical to those which are observed in AFM experiments. This model can be useful for numerical simulation of interaction of bacterium to the substrate.

## 3. Simulation Methodology and Basic Relationships

### 3.1. Movement of Bacterium

The Discrete Element Method (DEM) methodology based on the Lagrangian approach is applied to simulate dynamic behaviour of the bacterium under normal impact. Bacterium is considered as adhesive ultrafine particle. The motion of arbitrary bacterium  $i$  in time  $t$  during normal contact is characterized by the global parameters: positions  $\mathbf{x}_i$ , velocities  $\dot{\mathbf{x}}_i = d\mathbf{x}_i/dt$  and accelerations  $\ddot{\mathbf{x}}_i = d^2\mathbf{x}_i/dt^2$  of the mass center and a force  $\mathbf{F}_i$  applied to it. The global parameters are defined in Cartesian coordinates. Translational motion is described by the Newton's second law applied to each bacterium  $i$ :

$$m_i \ddot{\mathbf{x}}_i(t) = \mathbf{F}_i(t), \quad (1)$$

where  $m_i$  is the mass. The resultant force acting on the bacterium may comprise the prescribed as well as interaction and field forces. Consequently, for normal interaction, vector Equation (1) is reduced to scalar equation, while force vector is reduced to a single normal force  $F_i^N$ . Methodology of calculating the interaction forces in Equation (1) depends on the bacterium size, shape and mechanical properties as well as on the constitutive model of the interaction. The dynamical state of bacterium during interaction is tracked in space and time by integration of Equation (1). The numerical solution at the time  $t + \Delta t$  is obtained incrementally with constant time step  $\Delta t$  by using the 5<sup>th</sup>-order Gear predictor-corrector scheme. The discussed methodology was implemented into the original code.

### 3.2. Basic Models of Interaction

The constitutive model for normal adhesive contact of ultrafine bacterium on plane substrate is formulated based on the models of DMT and DLVO. These models involve the combined action of the repulsive contact force and attractive adhesive force. It should be noted that elastic contact is an extreme case of (stiff) deformable particle model, which will be applied to evaluate the upper bound of contact behaviour of bacterium.

For description bacterium behaviour we compare two introduced models. These models have different interpretation of deformation process. With the first model it is idealized that electrostatic double force is also acting during deformation and this process is described with time dependent double layer electrostatic force using Poisson-Boltzmann model. With the second model, it is assumed that contact is elastic and deformation is described with time dependent Hertz model. In both case at non contact deformation zone, when interacting surfaces are at the distance, interaction is described in same way, with time dependent attractive van der Waals and repulsive electrostatic double layer forces. Hydrodynamic and steric forces here are not assumed.

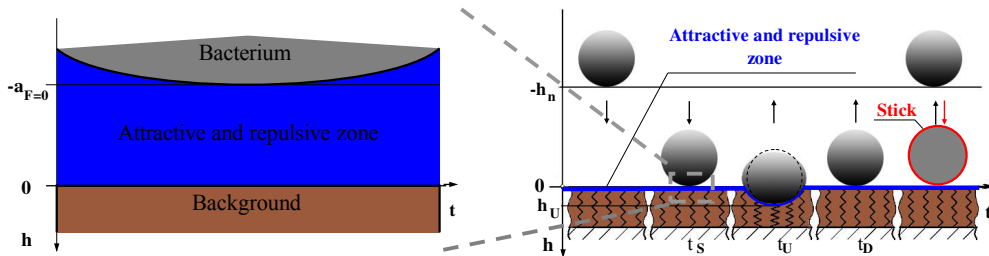


Fig. 1. Movement of bacterium

The movement of bacterium in time is illustrated by varying displacement  $h$  presented in Figure 1. Here negative positive displacement means interaction with contact deformation, while negative displacement means interaction without any contact deformation.

Firstly, bacterium, is moving from certain distance  $h_n$  to a surface. The short-range interaction-zone between particle and surface is denoted in Figure 1 presented with blue area which is limited by  $a_{F=0}$ . Our investigation is limited to bacterium interaction from time instance  $t_s$  till time instance  $t_D$ . It is assumed, that interaction starts at initial time period  $t_s$  when bacterium comes into the attractive and repulsive zone. In this work we investigate only interaction process and time instance  $t_s$  is assumed to be initial time  $t_0$ . Here particle has approach process with displacement  $h < 0$ . Basing on DLVO theory, this blue zone has attractive and repulsive behaviour manner. Attraction is basically related to van der Waals force. When particle reaches the surface with displacement  $h = 0$ , contact area of the interacting surfaces is under deformation and process is described as loading with displacement  $h > 0$ . During the contact at loading process of interacting surfaces, at period  $t_U$  bacterium reach maximum overlap displacement and rebound process begins. After that bacterium has unloading process with displacement  $h > 0$ . During unloading, when bacterium reach displacement distance  $h = 0$ , bacterium contact ends. At time period  $t_D$  bacterium is leaving attractive and repulsive zone and this process is described as detachment with displacement  $h < 0$ . If bacterium has not enough initial kinetic energy for rebound, interaction remains to bacterium sticking process to the interacting flat surface.

Bacterium interaction is described basing on known models by applying three different nature normal force components: attraction  $\mathbf{F}_{\text{attr}}^N(t)$ , repulsion  $\mathbf{F}_{\text{repulsion}}^N(t)$ , dissipation  $\mathbf{F}_{\text{diss}}^N(t)$ . Generally normal force of interaction can be described as a sum of these forces

$$\mathbf{F}^N(t) = \mathbf{F}_{\text{repulsion}}^N(t) + \mathbf{F}_{\text{attr}}^N(t) + \mathbf{F}_{\text{diss}}^N(t) \quad (2)$$

Different combination of these forces play significant role during bacterium approach, loading, unloading and detachment. Now will be introduced movement of bacterium.

#### 4. Basic Data of Simulation

In this work it is numerically investigated *S. aureus* bacterium interaction with glass surface, when initial distance between bacterium and glass surface is equal to  $a_{F=0} = 20$  nm. The diameter of bacterium is  $d = 1$   $\mu\text{m}$ , while density is  $\rho_i = 1.415$   $\text{g/cm}^3$ , Bakken and Olsen (1983) [24]. The density of a glass surface is  $\rho_j = 2.470$   $\text{g/cm}^3$ . During interaction of bacterium and a glass surface, bacterium is surrounded by water. Surface energy of bacterium is  $\gamma_A = 14.29$   $\text{mJ/m}^2$ , Hamadi et al. (2013) [25]. Elastic modulus of native *S. aureus* is  $1.33 \pm 0.21$  MPa, Jin et al. (2010) [26], and set as  $E_i = 0.0012$  GPa, Poissons coefficient is  $\nu_i = 0.5$ , Touhami et al. (2003) [27]. Elastic modulus of a glass is taken  $E_j = 80.1$  GPa, Poisson's coefficient is  $\nu_j = 0.27$ . The friction coefficient of bacterium and a glass surface is taken  $\mu = 0.05$ . For interaction in water pH 7, ionic strength is taken  $\sim 0.1$  M, Linke and Goldman (2011) [28]. The surface potentials of a glass surface and *S. aureus* are, respectively, -35 mV and -6 mV, Ducker et al. (1992) [29], Prince and Dickinson (2003) [30], Linke and Goldman (2011) [28]. Debbye length is chosen  $\lambda_D = 9.622$  nm. Boltzmann's constant  $k_B = 1.381 \cdot 10^{-23}$   $\text{J K}^{-1}$ . Dielectric constant of water  $\epsilon = 78.54$  at temperature 298 K, the permittivity of free space  $\epsilon_0 = 8.854 \cdot 10^{-12}$   $\text{C}^2 \text{J}^{-1} \text{m}^{-1}$ . The valence of electrolyte ions  $z = 1$  for NaCl and the charge of an electron  $e_c = 1.602 \cdot 10^{-19}$  C. The initial adhesion force is set as  $F_{L,adh}^N = 200$  pN, see H. Jin et al. (2010) [26], Touhami et al. (2004) [18]. By using these values in Equation (2) it is calculated the theoretical forces between *S. aureus* bacterium and a glass surface.

#### 5. Results

The results of present task show theoretical *S. aureus* bacterium behaviour during interaction with a glass surface. The theoretical interpretation of deformation behaviour of bacterium is till unknown, while it is meaningful interpretation of this process in order to understand the nature of bacterium interaction.

The results show different behaviour of bacterium using two models non elastic and elastic. Non elastic deformation model here described basing on electrostatic double layer forces, while the elastic contact is described using Hertz model. The comparison of these two (non elastic and elastic) models show the influence of the elastic deformation and the behaviour of the bacterium during the interaction process. Here the bacterium is interpreted as active colloid particle which has ability to be attracted to the surface by acting van der Waals forces. Non elastic model presented in figures with red line, while elastic with blue line.

Force displacement diagram is shown in Figure 2a, while time history of normal force is presented in Figure 2b. Here negative force means attraction, while positive repulsion. Positive displacement means interaction with contact deformation, while negative displacement means interaction without any contact deformation.

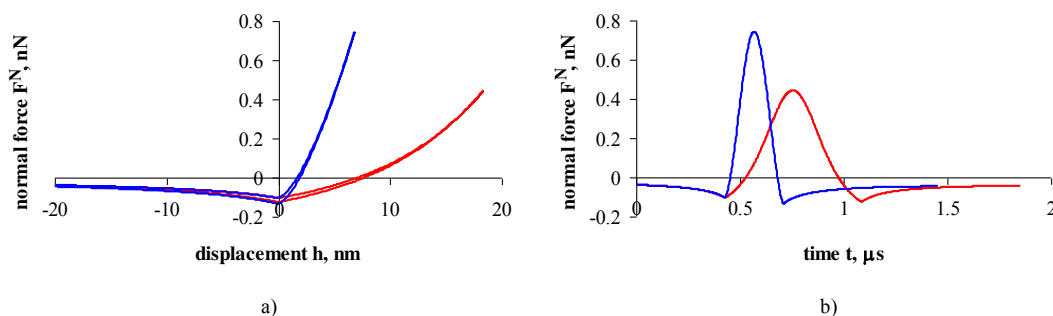


Fig.2. a) normal force  $F^N$  versus displacement  $h$ ; b) normal force  $F^N$  time history. Debye length  $\lambda_D = 9.61$ .

1 – deformation described with electrostatic double layer interaction (red line); 2 – deformation described with Hertz model (blue line).

The first Figure 2a shows hysteresis behaviour of the bacterium. During deformation different models show different behaviour of bacterium. Using Hertz model it is reached higher values of normal force. When deformation process is described with electrostatic double layer forces, during loading bacterium become more deformed, this

show displacement values. In both cases, during unloading and detachment the normal force is lower, it is because in presented models it is assumed increase of attractive forces because of surface roughness, see Tomas (2008) [31].

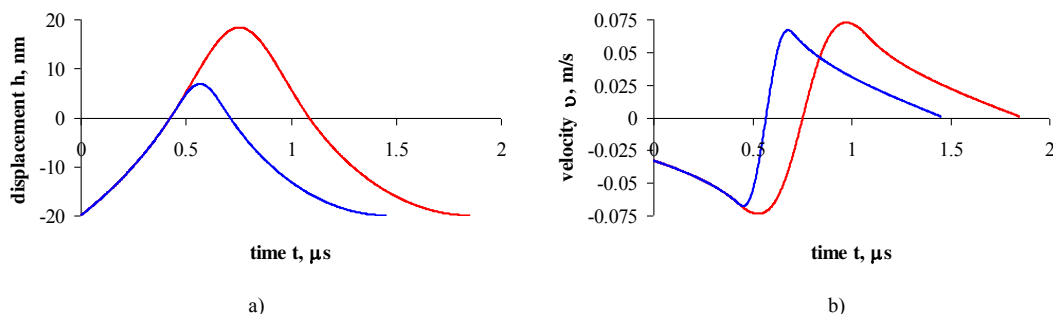


Fig.3. a) displacement  $h$  time history; b) velocity  $v$  time history. Debye length  $\lambda_D = 9.61$ .

1 – deformation described with electrostatic double layer interaction (red line); 2 – deformation described with Hertz model (blue line).

Time histories of displacement and velocities are presented in Figures 3a and 3b, respectively. With non elastic model bacterium reach higher values of displacement and velocity. The amount of dissipated energy during interaction was same as initial kinetic energy. The value of amount of dissipated energy was same for both models. In both cases during interaction all initial kinetic energy was dissipated.

During approach and detachment ( $h < 0$ ) for bacterium movement in liquid medium electrostatic force become not dominant and in both cases of models the approach and detachment remains with negative forces and attractive manner. The idealized non elastic model was described with electrostatic double layer force, while behaviour of bacterium becomes similar for behaviour of elastic-plastic particle. The duration of interaction for non elastic model become longer also the values maximum displacement increase, while force decrease. Basing on physical experiments with bacteria Touhami et al. (2004) [18], Abu-Lail et al. (2012) [19], Younes et al. (2012) [20], the results show that bacterium closer to elastic-plastic manner. Also the investigation needs comparison of bacterium deformation using known elastic-plastic models Tomas (2007) [21], Jasevičius et al. (2011) [22].

## 6. Conclusion

By applying known models for description of approach process the positive values of normal force was not reached and behaviour was of attractive manner. Otherwise the attractive manner is typical for interacting ultrafine objects.

DLVO model is usually used only for description of interaction without any contact deformation. The idealization and implementation of this model for description of deformation process the theoretical behaviour of bacterium become similar to behaviour of deformed body. Besides, the behaviour was closer to elastic-plastic manner, because in comparison with elastic Hertz model, the value of maximum displacement increase, while the value of maximum force decrease, also interaction duration become longer. The implemented energy dissipation mechanism related to adhesion agrees with DLVO, DMT and Hertz models. In both presented models amount of dissipated energy was same and independent on initial velocity and type of the model. This is typical for non biological particles, while it can be applied for bacterium behaviour as one of important condition to create such as structures like biofilm.

Future experiments must be addressed to numerical investigation of bacterium elastic-plastic behaviour by applying theoretical models used for ultrafine particles.

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